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Positron-hydrogen atom scattering using two channel optical potential

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Abstract : A two channel optical potential model is employed to investigate positron-hydrogen scattering in which P-space contains the basis set {H $(1s,2s,2p)$ + Ps $(1s,2s,2p)$} and {H $(3\bar{s},3\bar{p},3\bar{d})$ + Ps $(3\bar{s},3\bar{p},3\bar{d})$} constitutes Q-space. The results for integrated elastic, Ps-formation and differential cross sections are found to be very encouraging when compared with reliable existing theoretical predictions and available measured values in the energy range 54.4 to 100 eV.

Keywords : Positron-hydrogen atom scattering, optical potential

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1. Introduction

Literature reveals that the scattering cross section for positron-atom scattering is very slowly convergent with added eigen or pseudo states. Moreover, reliable cross section is very difficult to obtain at medium energies where an infinite number of channels are open. In the case of hydrogen as a target, a large number of reliable calculations [1–4] have been carried out. It is believed that elastic cross section of e^+-H scattering is now known to better than 10% at any energy [5]. For heavier target, this is not true. It becomes necessary to adopt a tractable model in which the effect of the higher excited states and continuum omitted in a truncated close coupling method (CCA), is taken into account. The optical potential method [6–9] meets this requirement partially. This method was applied to positron-hydrogen scattering by Bransden *et al* [9]. In their calculation, they have neglected the positronium (Ps) formation channel. Ghosh and Darewych [10] have suggested a method to include Ps formation channel in the framework of optical potential method as proposed by McCarthy and his co-authors.

Here, we apply an optical potential method as suggested by Ghosh and Darewych to investigate positron-hydrogen scattering. There are some elaborate calculations using multi-pseudo state CCA for this system. Walters [1] has studied positron-hydrogen scattering using a single channel close coupled pseudostate approximation. He has included the states upto $l \leq 2$ in the basis set and target states of higher angular momentum are treated perturbatively. Kernoghan *et al* [5] have employed an 18-state two channel pseudostate CCA to investigate the problem. The results of Kernoghan *et al* are expected to be more reliable than those of Walters [1] and Mitroy and Ratnavelu [4]. The purpose of the present work is to find the suitability of the present two channel optical potential model by comparing the present results with existing reliable theoretical predictions and available measured data.

2. Theory

The total space of the reaction channel is partitioned into two complementary sub spaces P and Q. P-space contains the basis set consisting of H $(1s,2s,2p)$ and Ps $(1s,2s,2p)$. The remaining channels including continuum are approximated by H $(3\bar{s},3\bar{p},3\bar{d})$ and Ps $(3\bar{s},3\bar{p},3\bar{d})$. Here bar denotes pseudostates.

The optical potential which is non-local, energy-dependent and complex in nature, are obtained following the method of Bransden *et al* and Ghosh and Darewych. With the optical potential, the Schrödinger equation for P-space are solved exactly.

The resulting coupled integral equations for the scattering amplitude [10] in the framework of optical potential formalism, are of the form :

$$f_{\beta\alpha}(k'n'_\beta;kn_\alpha) = f^Q_{\beta\alpha}(k'n'_\beta;kn_\alpha) - (1/2\pi^2)\sum_\gamma \sum_{n''_\gamma \epsilon P} \int dk''(k^2_{n''_\gamma} - k''^2 + i\varepsilon)^{-1}$$

$$f^Q_{\beta\gamma}(k'n'_\beta;k''n''_\gamma) f_{\gamma\alpha}(k''n''_\gamma;kn_\alpha).$$

Here (α,β) stands for the channels and $f^B_{\beta\alpha}$ is the scattering amplitude involving the interaction potential and optical potential and is given by

$$f^Q_{\beta\alpha}(k'n';kn) = f^B_{\beta\alpha}(k'n'_\beta;kn_\alpha) - (1/2\pi^2)\sum_{n''_\gamma \epsilon Q} \int dk''(k^2_{n''_\gamma} - k''^2 + i\varepsilon)^{-1}$$

$$\times f^B_{\beta\gamma}(k'n'_\beta;k''n''_\gamma) f^B_{\gamma\alpha}(k''n''_\gamma;kn_\alpha).$$

Here $f^B_{\beta\alpha}$ is the first Born scattering amplitude. We assume that state vectors of Q-space are plane waves and the coupling of the channels is the Q-space with each other is neglected. Moreover, in obtaining the optical potential scattering amplitude we retain upto second order term. These assumptions are also made by McCarthy and Stelbovics [6,7] and Bransden *et al* [9].

3. Results and discussions

In the present study, the pseudo-states are taken from Burke and Webb [11] and Dumburg and Karule [12]. Here, we develope a numerical code to solve the coupled integral equation. This code reproduces the 6-state CCA results of Sarkar *et al*. Inclusion of $3\bar{p}$ and $3\bar{d}$

pseudo-states allows to incorporate the dipole and quadrupole effects completely. Our results are found to be moderately convergent with the added pseudo-states. It may be noted that $f^B_{\beta\alpha}$ is either purely real or purely imaginary, whereas $f^Q_{\beta\alpha}$ is always complex.

We report results for positron scattering by ground state hydrogen atom in the energy range 54.4 to 200 eV. We present elastic, positronium formation and excitation

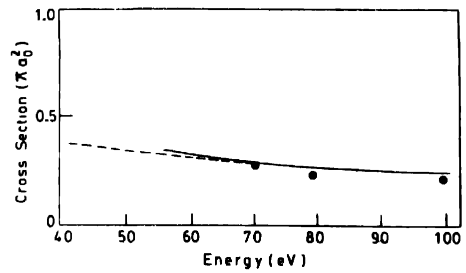

Figure 1. Total elastic cross sections for e^+-H scattering at different energies : solid line, present results; broken line, results of Kernoghan *et al* [5], and solid circles, results of Walters [1].

cross sections (2*s*- and 2*p*-state of target atom). The elastic integrated cross sections are presented in Figure 1 along with the corresponding predictions of Walters [1] and Kernoghan *et al* [5]. (6+6)-state CCA calculations have been carried out by Mitroy and Ratnavelu [4]. We cannot compare our results with those of them [4] as they have only reported low energy results. Therefore, we compare our results with most reliable calculations of Kernoghan *et al* [5]. The present results are in good agreement with those of Kernoghan *et al* in the incident energies considered. Our results coalesce with those [5] above 70 eV. The prediction of Walters are also in fair agreement with those of ours in the energy range considered. In Table 1, we compare our integrated 2*s*- and 2*p*-excitation cross

Table 1. Integrated 2*s*- and 2*p*-excitation cross sections for e^+-H scattering in unit of πa_0^2.

Energy (eV)	Integrated cross sections			
	1*s*–2*s*		1*s*–2*p*	
	Present	Walters	Present	Walters
54.4	0.095	0.127	0.93	0.95
100 0	0.058	0.061	0.73	0.71
200.0	0.028	0.03	0.48	0.47

sections with those of Walters. At 54.4 eV, the difference between the present integrated 2*s*-excitation cross section and those of Walters is almost 30%, his prediction being higher. At higher energies, they are in good agreement. In the case of 2*p*-excitation cross section, two sets of results are very close to each other in the energy range considered.

We define the total Ps-formation cross section as

$$\sigma^T_{\mathrm{Ps}} = \sigma^{\mathrm{el}}_{\mathrm{Ps}} + \sigma^{\mathrm{ex}}_{\mathrm{Ps}}(2s) + \sigma^{\mathrm{ex}}_{\mathrm{Ps}}(2p).$$

The present results in the energy range 54.4 to 100 eV are compared with measured data and the theoretical predictions of Kernoghan *et al* in Figure 2. The present optical potential

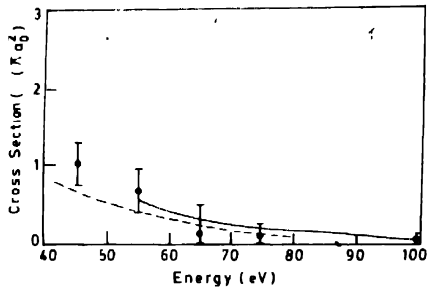

Figure 2. Total positronium formation cross sections for e^+-H scattering at different energies solid line, present results, broken line, results of Kernoghan *et al* [5], solid circles with error bars are the results of Weber *et al* [14].

results are in good accord with measured data in the energy range considered. The present total Ps-formation cross sections are also in fair agreement with those of 18-state calculation of Kernoghan *et al.* However, the results of Kernoghan *et al* are theoretically more sound than those of ours.

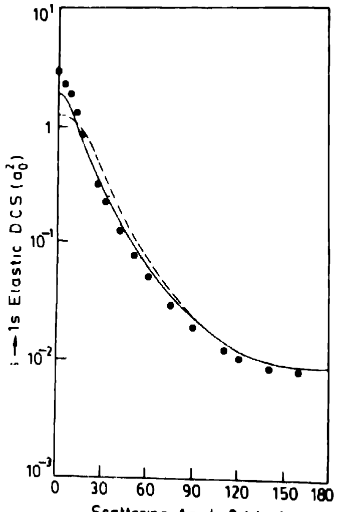

Figure 3. Differential elastic (1*s*–1*s*) cross sections for e^+-H scattering at 54.4 eV · solid line, present results; broken line, the results of Sarkar *et al* [13]; and solid circles are the results of Walters [1].

In Figures 3–5, we display the present differential cross sections (dc) for elastic, 2*s*- and 2*p*-excitations at 54.4 eV. Our elastic differential cross sections (dcs) are in very good accord with those of Walters except very near the forward direction. The elastic dc's near the forward direction is higher than the 6-state CCA prediction of Sarkar *et al.* On the

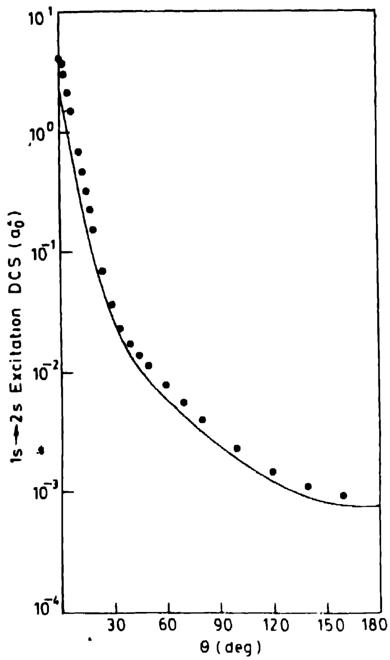

Figure 4. Differential excitation ($1s$–$2s$) cross sections for e^+-H scattering at 54.4 eV : solid line, present results, solid circles are the results of Walters [1]

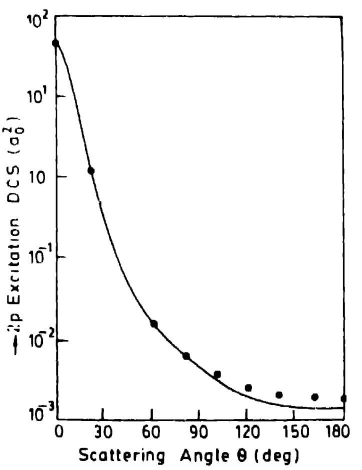

Figure 5. Differential excitation ($1s$–$2p$) cross sections for e^+-H scattering at 54.4 eV solid line, present results; and the solid circles are the results of Walters [1].

otherhand, the present dcs near the forward direction is less than that of Walters. By comparing our results, near the forward direction with those of 6-state calculation of Sarkar *et al*, it may be concluded that dc's near the forward direction is enhanced by the inclusion of the optical potential. The dc's near the forward direction of Walters *et al* suggests that the present model fails to include totally the loss of inelastic flux. However, this model include the loss of inelastic flux significantly as it is evident from the Figure. The present dc's for $2s$-excitation (Figure 4) have the same feature when compared with those of Walters and Sarkar *et al* (not shown here). However, $2p$-excitation dc's are in very good agreement with those of Walters and Sarkar *et al* (not shown here). With the increase of energy, the present optical potential results are found to agree well with those of Walters and Sarkar *et al* (not shown here).

Our main motivation is to find the suitability of the present model. We compare our results with most elaborate and reliable predictions just to find the accuracy of our model. The present findings have amply established this fact. The two-channel optical potential model is found to be reliable in yielding reliable results at medium energies.

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